Photonic Band Structure Calculation of 3D-Finite Nanostructured Supercrystals

José Luis Montaño-Priede[1]
Nicolas Large[2*]

1 Department of Electricity and Electronics, FCT-ZTF, UPV-EHU, 48080 Bilbao, Spain
2 Department of Physics and Astronomy, The University of Texas at San Antonio, One UTSA circle, San Antonio, Texas 78249, United States

joseluis.montano@ehu.eus
Nicolas.Large@utsa.edu

Abstract

In the last decades, plasmonic nanostructures have made possible the miniaturisation of photonic devises such as photonic crystals for sensing, photonic integrated circuits, etc. [1,2] The light-matter interaction in such supercrystals (Figure 1) are dependent in the lattice type, particle size, shape, and composition, as well as microcrystal habit. With the countless superlattices now synthetically realizable, computational methods and theoretical models play a crucial role in identifying the supercrystals that exhibit the most exciting properties. To tackle this problem, two approaches are generally taken (i) an effective medium theory approach which neglects the nanoscale effects to focus on the overall optical properties of the supercrystal, and (ii) the use of a unit cell with periodic boundary conditions which neglect the overall habit of the supercrystal to focus on nanoscale behaviour. This second approach is used for the calculation of the photonic band structure of these periodic structures. However, it fails to describe the photonic properties rising from finite-size effects such as Fabry-Pérot resonances. Here, we developed a computational approach, based on FDTD electrodynamic method to accurately calculate the photonic band structures from finite, microscale 3D supercrystals of cubic, spherical, and rhombic dodecahedral habits.

References

[1] Niclas S. Mueller et al. Nature, 583 (2020) 780–784
[2] Michael B. Ross et al. Nature Nanotechnology, 10 (2015) 453-458

Figures

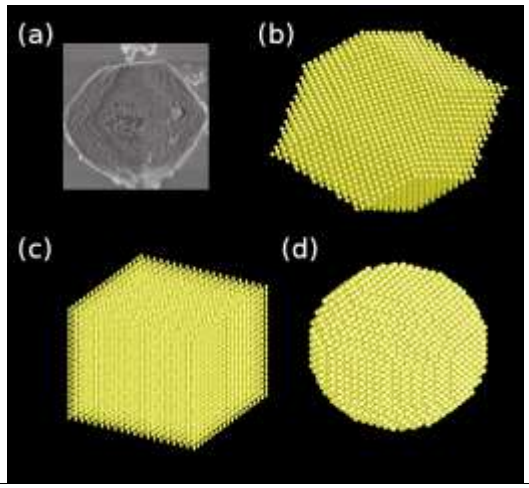

Figure 1: (a) SEM image of Au-nanoparticle rhombic-dodecahedral supercrystal [2]. (b)-(c) Au nanoparticle supercrystals with rhombic dodecahedral, cubic, and spheric habits

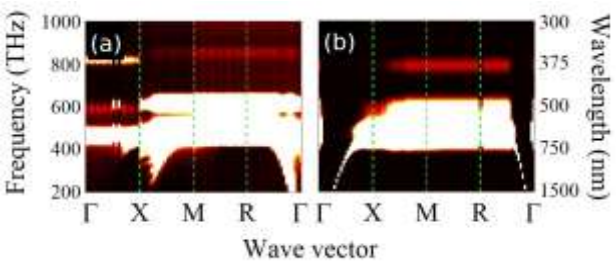

Figure 1: Photonic band structures of a (a) finite cubic lattice supercrystal with cubic habit of 2 um in length and (b) infinite cubic lattice supercrystal both with distance of 20 nm between spherical 80-nm Au NPs